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Boron and nitrogen-doped single-walled carbon nanotube

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Abstract

Boron nitride semiconducting zigzag single-walled carbon nanotube (SWCNT), $B_{cb}N_{cn}C_{1-cb-cn}$, as a potential candidate for making nanoelectronic devices is investigated by first-principle full potential density functional theory (DFT). In contrast to the previous DFT calculations, where just one boron and nitrogen doping configuration is considered, here for the average over all possible configurations density of states is calculated in terms of boron and nitrogen concentrations. For example in many body techniques (MBTs) [R. Moradian, Phys. Rev. B 89 (2004) 205425] it is found that semiconducting average gap, E_g, could be controlled by doping nitrogen and boron. But in contrast to MBTs where gap edge in the average density of states is sharp, the gap edge is smeared and impurity states appear in the SWCNT semiconducting gap.

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1. Introduction

Electronic structure of a single-walled carbon nanotube (SWCNT) can be determined in terms of chiral wrapping vector (n, m). For $(2n + m)/3 = integer$, SWCNTs are metallic and others are semiconductors [1,2]. A SWCNT with $m = n$ and 0 is called *armchair* and *zigzag*, respectively, and others are known as *chiral* SWCNT. For big enough diameter SWCNTs, armchair SWCNTs are always metallic. A zigzag carbon nanotube $(n, 0)$, is a semiconductor when $n/3 \neq integer$. Such semiconductor zigzag carbon nanotubes have the ability to become base of many nanoelectronic devices. Fabrication of nanoelectronic devices using carbon nanotubes is interesting due to the technological applications. By substitutional doping of boron and nitrogen, it is possible to provide more control on electronic properties of a semiconducting SWCNT [3–5]. It has been shown that the isolated nitrogen impurity forms a flat energy level lying inside the band gap [5]. Using effective medium super-cell approximation (EMSCA) technique [6,7], it has been found that the energy gap E_g of a semiconductor zigzag SWCNT can be changed by implanting boron and nitrogen [3]. In all the works done by DFT methods for investigation of boron nitride alloys, $B_{cb}N_{cn}C_{1-cb-cn}$, just one of the configurations has been considered [5,8–10], while measurable quantities are related to the statistical configurational average of such quantities, which included all the configurations' contribution. Our task is to investigate a boron nitride semiconducting zigzag SWCNT using first-principle full potential density functional theory where for the first time all possible impurity configurations are considered by this technique. This paper is organized as follows: in Section 2 we describe formalism and statistical averaged calculation method of density of states. In Sections 3 and 4 we illustrate our results and conclusions.

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2. Calculation formalism

Here we investigate a boron nitride semiconducting zigzag (10, 0) SWCNT alloy, $B_{cb}N_{cn}C_{1-cb-cn}$ within first-principle full potential linearized augmented plane-wave density functional theory as implemented in the WIEN2k code [11]. For the exchange and correlation terms the generalized gradient approximation (GGA) is used in the following [12]. For carbon, boron and nitrogen atoms the 1s state is the core state while 2s and 2p are the valance states. Muffin-tin radii of 1.3 a.u are used. The total number of k points in the whole Brillouin zone (BZ) is 200. Calculations are performed in the super-cell approximation with hexagonal unit cell. Length of the super-cell is 20 Å in the x, y-directions and $3 \times 4.267\,\text{Å} = 12.801\,\text{Å}$ along the tube axis (z-direction). Equilibrium positions of all atoms are determined using damped Newton dynamics method. Our chosen super-cell includes $N_s = 120$ atoms with periodic boundary conditions and the tubes are arranged parallel to the z-axis and form a triangular lattice in the perpendicular x–y plane; to avoid interaction between SWCNTs in such a lattice we have chosen large parameters in the $x-y$ plane. In the substitution doping of SWCNT super-cell by nitrogen and boron there are 3^{N_s} different configurations. For calculation of average quantities, contribution of each configuration should be considered with its probability. This was not considered previously in the DFT calculations for boron and nitrogen doping [5,10]. The probability of occupying a lattice site in a $B_{cb}N_{cn}C_{1-cb-cn}$ SWCNT, by a boron, a nitrogen and a carbon is given by cb, cn and $1 - cb - cn$, respectively. Thus, for a super-cell the probability of a given configuration, α, with N_1 boron atoms and N_2 nitrogen atoms is

$$P(\alpha) = cb^{N_1} cn^{N_2} (1 - cb - cn)^{N_s - N_1 - N_2}. \quad (1)$$

The configurational average of a physical quantity, $X_i^{\alpha}(E)$, at a given site i is defined by

$$\bar{X}_i(E) = \sum_{\alpha=1}^{3^{N_s}} P(\alpha) X_i^{\alpha}(E). \quad (2)$$

Since we restrict ourselves to the low impurity doping, keeping all possible 3^{120} configurations is not necessary. At low boron and nitrogen concentrations, configurations with no boron and one nitrogen atom (called $\alpha = 1$), no nitrogen and one boron atom (called $\alpha = 2$), or no boron and no nitrogen atoms (called $\alpha = 3$) mainly contribute to the averaging. So the average density of states is given by

$$\begin{aligned}\bar{N}_i(E) = {} & N_s cn(1 - cb - cn)^{N_s - 1} N_i^1(E) \\ & + N_s cb(1 - cb - cn)^{N_s - 1} N_i^2(E) \\ & + (1 - cb - cn)^{N_s} N_i^3(E). \end{aligned} \quad (3)$$

To calculate average density of states in Eq. (3), $N_i^3(E)$, $N_i^2(E)$, $N_i^1(E)$ should be calculated. Fig. 1 shows density of states components, $N_i^3(E)$, $N_i^2(E)$, $N_i^1(E)$, respectively. In the next section we shall illustrate our results.

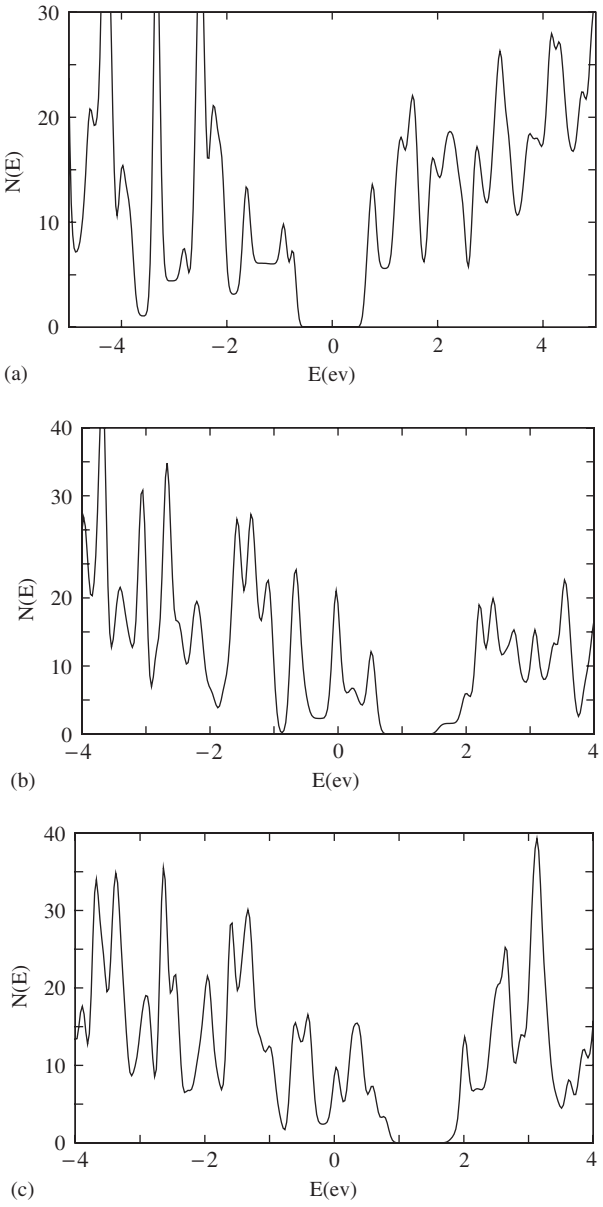

Fig. 1. Density of states of (a) a (10, 0) zigzag single-wall carbon nanotube, (b) where one of the carbon atoms are substituted by a nitrogen atom in super-cell which included 120 carbon atoms (0.83% nitrogen doping), (c) where one of the carbon atoms are substituted by a boron atom (0.83% boron doping).

3. Results and discussion

To investigate details of influence of boron and nitrogen doping on a zigzag SWCNT, two cases are considered: first, boron concentration is fixed but nitrogen concentrations are varied. In the second case nitrogen concentration is fixed while boron concentrations are varied. For different boron and nitrogen concentrations the calculated density of states are compared.

Now we perform our calculations for the first case. Fig. 2(a) illustrates the effects of nitrogen doping on the average density of states of a (10, 0) zigzag SWCNT for two